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HEAT CONDUCTION THROUGH PERIODIC ARRAYS OF SPHERES

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Abstract—A boundary integral method for determining the effective conductivity of a periodic array of spheres embedded in a conducting matrix is described. The method is independent of the multipole expansion methods previously applied to this problem. The effective conductivities of simple cubic, body-centered cubic, and face-centered cubic arrays of perfectly conducting spheres are calculated. The results verify those of multipole expansion methods and demonstrate that boundary integral techniques may be successfully applied to problems involving periodic arrays of spheres.

NOMENCLATURE

a_j,	set of unknown coefficients, equation (22);
$A(\mathbf{y})$,	a function of $\mathbf{y}$, equation (16);
A_{lj},	stiffness matrix, equation (24);
c,	volume concentration of spheres;
D,	region within the sphere at the origin;
∂D,	surface of the sphere at the origin;
E,	matrix region within the unit cell at the origin;
$f(\mathbf{x})$,	surface flux, equation (14);
$F_m^n(z)$,	a function of z, equation (32);
$\mathbf{G}$,	overall temperature gradient;
i,	the unit imaginary number;
$j_n(z)$,	nth spherical Bessel function of the first kind;
$\mathbf{k}^\alpha$,	vector α of the reciprocal lattice;
$\mathbf{n}(\mathbf{x})$,	unit outward normal vector;
N,	number of unknowns;
$P_n^m(z)$,	associated Legendre function of the first kind;
$\mathbf{q}_m(\mathbf{x})$,	heat flux within the matrix;
$\mathbf{q}_s(\mathbf{x})$,	heat flux within the spheres;
$\mathbf{Q}$,	overall heat flux;
$\mathbf{r}^\alpha$,	position of sphere α;
$t(\mathbf{x}, \mathbf{y})$,	fundamental singular solution;
$T(\mathbf{x})$,	temperature;
U,	region within unit cell;
∂U,	surface of unit cell;
W_l,	forcing vector, equation (25);
$\mathbf{x}, \mathbf{y}$,	position vectors;
$Y_n^m(\theta, \phi)$,	surface harmonic function of the first kind;
$\mathbf{z}$,	an arbitrary vector.

Greek symbols

γ,	conductivity of spheres relative to matrix;
$\delta(\mathbf{x})$,	Dirac delta function;
θ,	axial angle;
κ,	effective conductivity relative to matrix;
τ,	volume of unit cell;
ϕ,	azimuthal angle;
$\phi_j(\mathbf{x})$,	basis functions, equation (22).

1. INTRODUCTION

THE PROBLEM of calculating the effective conductivity of a composite medium consisting of an array of spheres embedded in an isotropic matrix has been studied for many years. Rayleigh [1] was the first to offer a solution to this problem. His solution was later corrected by Runge [2] and improved by Meredith and Tobias [3]. Rayleigh's method of dealing with a non-convergent sum was questioned by Levine [4] and Jeffrey [5], leading to further work by a number of researchers [6–9]. These studies all used Rayleigh's basic technique of expressing the temperature field as a multipole expansion about each sphere; solutions accurate to higher concentrations of the spheres required higher ordered multipoles. O'Brien's paper was unique in that it also offered a method for calculating the effective conductivity of a dilute random suspension of particles. Keller [10] and Batchelor and O'Brien [11] have given asymptotic solutions for arrays in which the spheres were nearly touching.

The most complete solutions to this problem to date are provided by McPhedran and McKenzie [7] for the case of simple cubic arrays and McKenzie *et al.* [8] for body-centered and face-centered cubic arrays (these two papers will be henceforth referred to collectively as McKenzie *et al.* [7, 8]). Although their method of calculating the expansion coefficients for the body-centered and face-centered cubic arrays differs slightly from their method for the simple cubic case, McKenzie *et al.* [7, 8] have used high-ordered multipole expansions for the temperature fields in all of their work. The purpose of this paper is not to improve upon the work of McKenzie *et al.* Rather, it will offer a new method of solution for this problem, a method which does not use multipole expansions for the temperature field. This new method will then be used to corroborate the results of McKenzie *et al.* [7, 8].

The method of solution presented in this study is similar to the method employed by Zick and Homsy [12] to study Stokes flow through periodic arrays of spheres. Doubtless there are a number of other problems involving periodic arrays of spheres for which this method would also be useful. It is basically a boundary integral method. A periodic fundamental singular solution to the problem is first attained. This fundamental solution is then used to transform the set of governing differential equations and their associated boundary conditions into an integral equation with the surface of a single sphere as its domain. A Galerkin technique is then used to solve the integral equation numerically.

The boundary integral method is used to calculate the effective conductivities of perfectly conducting spheres in simple cubic, body-centered cubic, and face-centered cubic arrays at concentrations up to 95% of the maximum concentration for each type of array. The results agree with, and thus confirm by an independent technique, those of McKenzie *et al.* [7, 8].

2. FORMULATION OF PROBLEM

Consider a homogeneous matrix with unit conductivity surrounding a regular array of spheres having unit radius and conductivity γ. It is desired to determine the overall flux, $\mathbf{Q}$, and hence the effective conductivity, κ, when a temperature gradient, $\mathbf{G}$, is imposed on the lattice. Within the matrix

$$\mathbf{q}_m = -\nabla T, \tag{1}$$

$$\nabla \cdot \mathbf{q}_m = 0. \tag{2}$$

Within the spheres

$$\mathbf{q}_s = -\gamma \nabla T, \tag{3}$$

$$\nabla \cdot \mathbf{q}_s = 0. \tag{4}$$

On the surface of each sphere

$$\mathbf{n} \cdot \mathbf{q}_m = \mathbf{n} \cdot \mathbf{q}_s \tag{5}$$

where $\mathbf{n}$ is the outward unit normal vector. Also, except for the overall temperature gradient, the temperature is periodic, i.e.

$$T(\mathbf{x}+\mathbf{r}^\alpha) = T(\mathbf{x}) + \mathbf{G}\cdot\mathbf{r}^\alpha. \tag{6}$$

Here $\mathbf{r}^\alpha$ is the position vector of sphere α, $\alpha = 0, 1, 2, \ldots, \infty$, with $\mathbf{r}^0 = \mathbf{0}$. Finally, the temperature may be specified at one point; for simplicity we take

$$T(\mathbf{0}) = 0. \tag{7}$$

It is now assumed that each sphere within the lattice is indistinguishable from any other sphere. Since the problem is periodic, it is only necessary to consider a single unit cell of the array. For simplicity, we choose the one which is centered at the origin and which fully encloses the sphere at the origin. We define this unit cell as U and the surface of U as ∂U. Denoting the volume of the unit cell as τ, we note that the volume concentration of spheres, c, is given by

$$c = \frac{4\pi}{3\tau}. \tag{8}$$

The fundamental singular solution of this problem $t(\mathbf{x}, \mathbf{y})$, is the temperature field at position $\mathbf{x}$ due to an array of point sources centered at position $\mathbf{y}$ and it satisfies

$$\nabla^2 t(\mathbf{x},\mathbf{y}) = \frac{1}{\tau} - \sum_{\alpha=0}^{\infty} \delta(\mathbf{x}-\mathbf{y}-\mathbf{r}^\alpha). \tag{9}$$

The solution to this equation which has zero mean within a unit cell is

$$t(\mathbf{x},\mathbf{y}) = \frac{1}{4\pi^2\tau}\sum_{\alpha=1}^{\infty} |\mathbf{k}^\alpha|^{-2} e^{2\pi i \mathbf{k}^\alpha\cdot(\mathbf{x}-\mathbf{y})} \tag{10}$$

where $\mathbf{k}^\alpha$ is a non-zero reciprocal lattice vector [12, 13].

Define D to be the region within the sphere at the origin and ∂D to be the surface of that sphere. Then define E to be the matrix region external to D but within U. With use of the divergence theorem, two integral relations can be written,

$$\begin{aligned}\iiint_E &[T(x)\nabla^2 t(\mathbf{x},\mathbf{y}) - t(\mathbf{x},\mathbf{y})\nabla^2 T(\mathbf{x})]\,d\mathbf{x} \\ &= \iint_{\partial U} [T(\mathbf{x})\nabla t(\mathbf{x},\mathbf{y}) - t(\mathbf{x},\mathbf{y})\nabla T(\mathbf{x})]\cdot\mathbf{n}\,d\mathbf{x} \\ &\quad - \iint_{\partial D} [T(\mathbf{x})\nabla t(\mathbf{x},\mathbf{y}) - t(\mathbf{x},\mathbf{y})\nabla T(\mathbf{x})]\cdot\mathbf{n}\,d\mathbf{x}\end{aligned} \tag{11}$$

and

$$\begin{aligned}\iiint_D &[T(\mathbf{x})\nabla^2 t(\mathbf{x},\mathbf{y}) - t(\mathbf{x},\mathbf{y})\nabla^2 T(\mathbf{x})]\,d\mathbf{x} \\ &= \iint_{\partial D} [T(\mathbf{x})\nabla t(\mathbf{x},\mathbf{y}) - t(\mathbf{x},\mathbf{y})\nabla T(\mathbf{x})]\cdot\mathbf{n}\,d\mathbf{x}.\end{aligned} \tag{12}$$

By adding equations (11) and (12) and making use of equations (1)–(10) it can be shown that

$$T(\mathbf{y}) = \mathbf{G}\cdot\mathbf{y} + \iint_{\partial D} t(\mathbf{x},\mathbf{y}) f(\mathbf{x})\,d\mathbf{x} \tag{13}$$

where

$$f(\mathbf{x}) \equiv \left(1 - \frac{1}{\gamma}\right)\mathbf{q}_m(\mathbf{x})\cdot\mathbf{n}(\mathbf{x}) \tag{14}$$

shall be referred to as the surface flux.

By multiplying equation (12) by γ and adding it to equation (11) it can similarly be shown that

$$A(\mathbf{y})T(\mathbf{y}) = \mathbf{G}\cdot\mathbf{y} + (1-\gamma)\iint_{\partial D} \mathbf{n}\cdot\nabla t(\mathbf{x},\mathbf{y})T(\mathbf{x})\,d\mathbf{x} \tag{15}$$

where

$$A(\mathbf{y}) = \begin{cases} 1, & \mathbf{y}\in E, \\ \gamma, & \mathbf{y}\in D, \\ \tfrac{1}{2}(1+\gamma), & \mathbf{y}\in\partial D. \end{cases} \tag{16}$$

Equations (13)–(16) now present the problem in integral form. The desired quantity, namely the effective conductivity, κ, is given by

$$\kappa = \frac{-\mathbf{G}}{|\mathbf{G}|^2}\cdot\frac{1}{\tau}\left[\iiint_E \mathbf{q}_m(\mathbf{x})\,d\mathbf{x} + \iiint_D \mathbf{q}_s(\mathbf{x})\,d\mathbf{x}\right], \tag{17a}$$

$$= 1 - \frac{1}{\tau}\frac{\mathbf{G}}{|\mathbf{G}|^2}\cdot\iint_{\partial D} \mathbf{x} f(\mathbf{x})\,d\mathbf{x}. \tag{17b}$$

In order to obtain the effective conductivity of the array of spheres it is necessary to solve equations (13)–(16) for the unknown surface flux, $f(\mathbf{x})$, and to then apply equation (17b).

Restrict $\mathbf{y}$ to be on ∂D. Then equations (13)–(16) become two Fredholm integral equations, one of the second kind and one of the first,

$$\frac{1}{2}\left(\frac{1+\gamma}{1-\gamma}\right)T(\mathbf{y}) = \frac{\mathbf{G}\cdot\mathbf{y}}{(1-\gamma)} + \iint_{\partial D} \mathbf{n}\cdot\nabla t(\mathbf{x},\mathbf{y})T(\mathbf{x})\,d\mathbf{x}, \quad \mathbf{y}\in\partial D, \tag{18}$$

$$0 = \mathbf{G}\cdot\mathbf{y} - T(\mathbf{y}) + \iint_{\partial D} t(\mathbf{x},\mathbf{y})f(\mathbf{x})\,d\mathbf{x}, \quad \mathbf{y}\in\partial D. \tag{19}$$

In principal, equation (18) can be solved for $T(\mathbf{y})$, $\mathbf{y}\in\partial D$, and then equation (19) can be solved for $f(\mathbf{x})$. In practice however, equation (18) is difficult to solve unless the spheres are perfectly conducting, i.e. $\gamma = \infty$. We will therefore limit ourselves to the case of perfectly conducting spheres.

3. METHOD OF SOLUTION FOR PERFECTLY CONDUCTING INCLUSIONS

In the case $\gamma = \infty$, equation (18) reduces to

$$T(\mathbf{y}) = 0, \quad \mathbf{y}\in\partial D \tag{20}$$

giving the physically obvious result that as $\gamma \to \infty$ the spheres become isothermal. Then equation (19) reduces to

$$\mathbf{G}\cdot\mathbf{y} = -\iint_{\partial D} t(\mathbf{x},\mathbf{y})f(\mathbf{x})\,d\mathbf{x}, \quad \mathbf{y}\in\partial D. \tag{21}$$

As shown by Zick and Homsy [12], integral equations such as equation (21) can be readily solved by a Galerkin technique. Let us expand $f(\mathbf{x})$ as a linear combination of basis functions, $\phi_j(\mathbf{x})$, which form a complete set over the domain ∂D.

$$f(\mathbf{x}) = \sum_{j=1}^{N} a_j\phi_j(\mathbf{x}). \tag{22}$$

It can be shown that the set of coefficients, a_j, is the solution to the system of linear algebraic equations

$$\sum_{j=1}^{N} A_{lj}a_j = W_l, \quad l = 1,2,\ldots,N \tag{23}$$

where

$$A_{lj} = \iint_{\partial D}\left[\iint_{\partial D} t(\mathbf{x},\mathbf{y})\phi_j(\mathbf{x})\,d\mathbf{x}\right]\phi_l(\mathbf{y})\,d\mathbf{y}, \tag{24a}$$

$$= \frac{1}{4\pi^2\tau}\sum_{\alpha=1}^{\infty}|\mathbf{k}^\alpha|^{-2}\iint_{\partial D} e^{-2\pi i\mathbf{k}^\alpha\cdot\mathbf{y}} \times \phi_l(\mathbf{y})\,d\mathbf{y}\iint_{\partial D} e^{2\pi i\mathbf{k}^\alpha\cdot\mathbf{x}}\phi_j(\mathbf{x})\,d\mathbf{x} \tag{24b}$$

and

$$W_l = -\iint_{\partial D} \mathbf{G}\cdot\mathbf{y}\,\phi_l(\mathbf{y})\,d\mathbf{y}. \tag{25}$$

The effective conductivity is then given by

$$\kappa = 1 + \frac{1}{\tau|\mathbf{G}|^2}\lim_{N\to\infty}\sum_{j=1}^{N} a_jW_j. \tag{26}$$

The basis functions appropriate for this problem are the surface harmonics of the first kind,

$$Y_n^m(\theta,\phi) = \begin{Bmatrix}\cos m\phi \\ \sin m\phi\end{Bmatrix} P_n^m(\cos\theta), \quad m \leqslant n. \tag{27}$$

Since only isotropic arrays will be considered here, the overall temperature gradient, $\mathbf{G}$, can be taken to be in the 1-direction without loss of generality and it becomes necessary to consider only the surface harmonics of the form

$$\cos 2m\phi P_{2n+1}^{2m}(\cos\theta) \tag{28}$$

where the 1-direction corresponds to $\theta = 0$. It is more convenient from a computational viewpoint, however, to recast the basis functions as follows:

$$\begin{aligned}\phi_1(\mathbf{x}) &= x_1,\\ \phi_2(\mathbf{x}) &= x_1^3,\\ \phi_3(\mathbf{x}) &= x_1x_2^2,\\ \phi_4(\mathbf{x}) &= x_1^5,\\ \phi_5(\mathbf{x}) &= x_1^3x_2^2,\\ \phi_6(\mathbf{x}) &= x_1x_2^4, \text{ etc.}\end{aligned} \tag{29}$$

With these basis functions, all of the integrations required to evaluate A_{lj} and W_l can be performed analytically. It can be shown that for any vector $\mathbf{z}$,

$$\iint_D e^{i\mathbf{z}\cdot\mathbf{n}}n_1^pn_2^qn_3^t\,d\mathbf{x} = 4\pi\sum_{j=0,1}^{p}\sum_{k=0,1}^{q}\sum_{l=0,1}^{t} \times \frac{p!}{j![(p-j)/2]!}\frac{q!}{k![(q-k)/2]!}\frac{t!}{l![(t-l)/2]!} \times \frac{z_1^jz_2^kz_3^l}{|\mathbf{z}|^{j+k+l}}F_{j+k+l}^{p+q+t}(|\mathbf{z}|) \tag{30}$$

where $\sum_{j=0,1}^{p}$ indicates a summation over the values

$$j = \begin{cases}0,2,4,\ldots,p & \text{for } p \text{ even,}\\ 1,3,5,\ldots,p & \text{for } p \text{ odd}\end{cases} \tag{31}$$

and

$$F_{2l}^{2m}(z) \equiv (i)^{2l}(2z)^{-(m-l)}j_{m+l}(z) \tag{32}$$

where $j_n(z)$ is the nth spherical Bessel function of the first kind.

4. RESULTS AND DISCUSSION

The effective conductivity was calculated for simple cubic, body-centered cubic, and face-centered cubic

Table 1. Convergence of effective conductivities

Packing	SC	BCC	FCC	SC	BCC	FCC
	Concentration					
Unknowns	0.200	0.300	0.400	0.500	0.650	0.705
1	1.750	2.286	3.000	4.00	6.57	8.2
3	1.756	2.290	3.011	5.18	7.35	8.6
6	1.756	2.292	3.023	5.52	8.46	10.4
10		2.292	3.023	5.73	8.74	11.2
15			3.023	5.83	8.89	11.3
21				5.85	8.94	11.3
28				5.86	8.97	11.3
36				5.88	8.95	11.7
45				5.86	8.93	11.3
55				5.84	8.92	11.3

arrays of perfectly conducting spheres with concentrations up to 95% of that at maximum packing. The number of unknowns, a_j, was limited to 55 where each calculation required 5 min of CPU time on an IBM 3033 computer. This number of unknowns corresponds to the surface flux approximation which makes use of all of the surface harmonics, Y_{2n+1}^{2m}, with $0 \leqslant m \leqslant n \leqslant 9$. Table 1 illustrates the convergence rates which were typical of the calculations, indicating the present results are convergent to better than 1%.

Presented in Table 2 are the effective conductivities computed in this study compared with those computed by McKenzie *et al.* [7, 8]. The results presented here agree very well with those of McKenzie *et al.* [7, 8], thus confirming their results by an independent method.

It was decided not to investigate the effective conductivities of arrays with concentrations greater than 95% of the maximum, as the convergence of the solution is slow near the maximum concentrations. At maximum concentration there is a singularity in the surface flux at the sphere-to-sphere contact points. Even at concentrations slightly below the maximum there are large peaks in the surface flux near the points where the spheres almost touch. Successful approximation of these peaks requires a large number of basis functions and it was felt that extending the results to higher concentrations would not be worth the additional cost, especially since those results would probably be no more accurate than the results of McKenzie *et al.* [7, 8].

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REFERENCES

1. Lord Rayleigh, On the influence of obstacles arranged in rectangular order on the properties of the medium, *Phil. Mag.* **34**, 481–502 (1892).
2. I. Runge, On the electrical conductivity of metallic aggregates, *Z. Tech. Phys.* **6**, 61–68 (1925).
3. R. E. Meredith and C. W. Tobias, Resistance to potential flow through a cubical array of spheres, *J. Appl. Phys.* **31**, 1270–1273 (1960).
4. H. Levine, The effective conductivity of a regular composite medium, *J. Inst. Maths. Applic.* **2**, 12–28 (1966).
5. D. J. Jeffrey, Conduction through a random suspension of spheres, *Proc. R. Soc.* **A335**, 355–367 (1973).
6. M. Zuzovsky and H. Brenner, Effective conductivities of composite materials composed of cubic arrangements of spherical particles embedded in an isotropic matrix. *J. Appl. Math. Phys.* **28**, 979–992 (1977).
7. R. C. McPhedran and D. R. McKenzie, The conductivity of lattices of spheres. I. The simple cubic lattice, *Proc. R. Soc.* **A359**, 45–63 (1978).
8. D. R. McKenzie, R. C. McPhedran and G. H. Derrick, The conductivity of lattices of spheres. II. The body-centered and face-centered cubic lattices, *Proc. R. Soc.* **A362**, 211–232 (1978).
9. R. W. O'Brien, A method for the calculation of the effective transport properties of suspensions of interacting particles, *J. Fluid Mech.* **91**, 17–39 (1979).
10. J. B. Keller, Conductivity of a medium containing a dense array of perfectly conducting spheres or cylinders or non-conducting cylinders. *J. Appl. Phys.* **34**, 991–993 (1963).
11. G. K. Batchelor and R. W. O'Brien, Thermal or electrical conduction through a granular material, *Proc. R. Soc.* **A355**, 313–333 (1977).
12. A. A. Zick and G. M. Homsy, Stokes flow through periodic arrays of spheres, *J. Fluid Mech.* **115**, 13–26 (1982).
13. H. Hasimoto, On the periodic fundamental solutions of the Stokes equations and their application to viscous flow past a cubic array of spheres. *J. Fluid Mech.* **5**, 317–328 (1959).

Table 2. Effective conductivities for cubic arrays of perfectly conducting spheres

	SC array		BCC array		FCC array	
Concentration	Present work	Previous results [7]	Present work	Previous results [8]	Present work	Previous results [8]
0.10	1.334	1.334	1.333	1.333	1.333	1.333
0.20	1.756	1.756	1.751	1.751	1.751	1.750
0.30	2.333	2.333	2.292	2.292	2.290	2.290
0.40	3.262	3.261	3.035	3.035	3.023	3.023
0.50	5.84	5.887	4.166	4.166	4.106	4.106
0.5236		∞				
0.60			6.339	6.341	5.969	5.972
0.65			8.92	9.026		
0.6802				∞		
0.705					11.3	11.48
0.7405						∞

CONDUCTION THERMIQUE ENTRE DES ARRANGEMENTS PERIODIQUES DE SPHERES

Résumé—Une méthode intégrale est décrite pour déterminer la conductivité effective d'un arrangement périodique de sphères noyées dans une matrice conductrice. La méthode est indépendante des méthodes de développement multipole précédemment appliquées à ce problème. On calcule les conductivités effectives d'arrangements cubiques simples, cubiques centrés et cubiques à faces centrées de sphères parfaitement conductrices. Les résultats vérifient ceux des méthodes de développement multipole et ils démontrent que les techniques intégrales limites peuvent être appliquées avec succès aux problèmes d'arrangements périodiques de sphères.

WÄRMELEITUNG DURCH PERIODISCHE KUGELANORDNUNGEN

Zusammenfassung—Ein Randwertintegrationsverfahren zur Bestimmung des effektiven Wärmeleitvermögens einer periodischen Kugelanordnung, die in einem leitenden Medium eingebettet ist, wird beschrieben. Das Verfahren ist unabhängig von den Verfahren mit Multipol-Reihenentwicklung die früher auf dieses Problem angewandt wurden. Das effektive Leitvermögen von einfachen kubischen, kubisch raumzentrierten und kubisch flächenzentrierten Anordnungen von ideal leitenden Kugeln wurde berechnet. Die Ergebnisse bestätigen jene der Multipol-Reihenentwicklungsvergahren und zeigen, daß Randwertintegrationsverfahren erfolgreich für Probleme mit periodischen Kugelanordnungen angewendet werden können.

ПЕРЕДАЧА ТЕПЛА ТЕПЛОПРОВОДНОСТЬЮ В ПЕРИОДИЧЕСКИХ РЕШЕТКАХ СФЕР

Аннотация — Эффективная теплопроводность периодической решетки сфер в проводящей матрице определяется с помощью интегрального граничного метода, не привлекая мультипольное разложение, применявшееся ранее для решения этой задачи. Рассчитана эффективная теплопроводность пространственно-центрированных простых и гранецентрированных кубических решеток идеально проводящих сфер. Результаты расчета сходятся с полученными по методу мультипольного разложения. Таким образом, граничные интегральные методы эффективны для решения задач, связанных с периодическими системами сфер.